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$LiNbO_3$ Plate Bonded to Quartz as a Substrate for High Frequency Wideband SAW Devices

Natalya Naumenko
National University of Science and Technology "MISIS"
Moscow, Russia
nnaumenko@ieee.org

Abstract— **Bonded wafers combining a thin LiNbO3 plate with a quartz substrate were studied numerically as potential substrate materials for high frequency wideband SAW devices. Longitudinal leaky waves propagating with velocities up to 7000 m/s were investigated, and the multilayered structure was optimized to combine high velocity, high electromechanical coupling and negligible propagation losses. In the optimized structures non-attenuated waves can propagate with velocities V=5500-6200 m/s and coupling up to 18%. Examples of simulated admittances of SAW resonators demonstrate that in some optimal $LiNbO_3$/quartz structures high quality factors Q>5000 can be achieved simultaneously at resonant and anti-resonant frequencies if duty factor of electrode structure varies between 0.48 and 0.65. Due to sufficiently large optimal plate and electrode thicknesses, 40% and 5% of a wavelength, respectively, the found structures can be employed in SAW resonators operating at high frequencies, up to 5 GHz.**

Keywords—wideband SAW filter, multilayered structure, lithium niobate, high frequency resonator.

I. Introduction

The next generation of communication systems imposes strong demand for high performance surface acoustic wave (SAW) filters. The general tendency of moving to higher frequencies followed by increasing density of operating frequency bands results in strong requirements to our-of-band rejection and steeper bandpass skirts for isolation of signals in neighboring channels. In addition, multiple applications result in diversity of filter performances, which cannot be satisfied if only conventional substrate materials are employed. Therefore, in recent years, multilayered structures are extensively studied as an alternative to single crystal substrates.

This paper is focused on the search of a multilayered substrate material for high-frequency wideband SAW filters. For example, such substrate is required to realize the tunable filter with wide tunable range [1]. Wideband SAW filters operating at 5 GHz or higher frequencies require substrate materials, which combine large electromechanical coupling factor with high velocity of acoustic wave. $LiNbO_3$ (LN) enables the highest electromechanical coupling compared to other SAW materials. If LN orientation is optimized to support propagation of a high-velocity SAW, it could be a good choice of a substrate material but generally such waves leak strongly into the substrate and attenuate. As a result, insertion losses grow and Q-factor of a SAW device degrades.

Leakage can be suppressed if acoustic wave is guided in a thin LN plate. Kadota [1] used the first-order anti-symmetric mode A_1 propagating in thin ZX-LN plate for design and fabrication of 5.44 GHz Lamb wave resonator with wide bandwidth of 12%. Due to low plate thickness, which was only 395 nm or 0.15 λ, where λ is the acoustic wavelength, the measured effective velocity in Lamb wave resonators exceeded 11,000 m/s with coupling k^2=20.3%. However, such extremely thin plates are not suitable for mass production of high frequency resonators because they are fragile.

Bonding of LN plate to a supporting substrate directly or via intermediate layers allows improving mechanical stability of a SAW resonator. In resonators arranged on such multilayered substrates called 'Solidly Mounted (SM) type' [2] or 'Hetero Acoustic Layer (HAL)' [3-4] resonators, acoustic waves change their characteristics with plate and electrode thicknesses. Multilayered structures with LN plates were investigated by few research groups as potential substrates for high performance wideband SAW filters [2-5].

An acoustic wave propagating along the surface of a multilayered structure leaks into supporting substrate and attenuates if it is faster than at least one of the bulk acoustic waves (BAWs) in a substrate material. Therefore, a reflector of few alternating high- and low acoustic impedance layers is usually introduced between a plate and a substrate to suppress leakage. The loss mechanisms in bonded wafers with low- or high-velocity substrates and the effect of isolating layers on the wave structure and leakage were studied in [6].

Kadota [2] reported SM type ladder filter with three resonators employing the shear horizontal (SH)-type wave. The filter was designed and fabricated on YX-LN plate bonded to a glass substrate, with a number of alternating SiO_2 and AlN layers sufficient to suppress radiation of SH wave into glass and their thicknesses optimized to obtain clean responses with no spurious between resonant and anti-resonant frequencies. Pt and Au electrodes provided sufficient reflectivity in resonators, due to high density of these metals.

In a similar SM type or HAL device reported in [3] the 3.6 μm thick LN plate was bonded to a silicon substrate, with six isolating layers between them. Though high performance ladder filter with measured bandwidth of 20% was fabricated, the described multilayered structure cannot be applied in high frequency resonators because of existing technological limitations on minimum electrode width and low velocity of SH mode (3650 – 3830 m/s).

High velocity longitudinal leaky SAWs (LLSAWs) propagating in X,Y+36°-LN bonded to a sapphire or AT-quartz substrate were investigated by Gomi [4]. In a resonator with LN plate thickness of 0.2 λ, the high velocity (V=6400 m/s) and high coupling (k^2=19.7%) were obtained but LLSAW leakage into the substrate was not suppressed and Q-factors of SAW resonators were too low for application of this structure in high performance SAW filters.

Optimization of LN orientation and the use of Pt as a high acoustic impedance layer, instead of AlN, allowed Kimura [5] to achieve higher impedance ratio of 71 dB for LLSAW propagating with velocity V=6035 m/s and k^2=24.7% in 3.5 GHz SM type resonators with the fractional bandwidth of 9.5%. However, with five isolating layers leakage was not totally suppressed and the measured Q-factor (Q=665) was not high.

In the multilayered structures mentioned above leakage of LLSAW was suppressed by introduction of a reflector between LN plate and a substrate. There exists another method to suppress the leakage. It takes into account the symmetry of combined materials and their anisotropy. The symmetry consideration supplemented by a rigorous numerical simulation of resonator admittances and extraction of propagation losses as functions of substrate orientation, as well as plate and metal thicknesses, was recently successfully applied to optimization of LLSAWs in LT/quartz [7] and allowed to find non-attenuated acoustic waves propagating with velocities about 5500 m/s and electromechanical coupling of 6.8% in resonators with Q factors up to 10^4. Hereafter, the same method is applied to LN/quartz.

II. Numerical Results and Discussion

The nature of a surface wave generated by an interdigital transducer (IDT) arranged on top of a layered structure depends on the ratio between its velocity and limiting BAW ("cut-off") velocities in a substrate [8]. If at least one of the limiting BAWs propagates slower than SAW, such surface wave leaks into the substrate and attenuates.

Propagation of LLSAW is accompanied by radiation of the slow and fast quasi-shear (further called "shear", for simplicity) BAWs because these BAWs are slower than LLSAW. Attenuation of LLSAW is usually higher than attenuation of a low-velocity LSAW, which propagates faster than the slow shear BAW but slower than the fast shear BAW. However, leakage of the high-velocity SAW can be reduced if one of the BAWs is uncoupled with dominant polarization of the wave, due to crystal symmetry. Further suppression of leakage can be achieved via optimization of a substrate orientation, if a substrate with strong elastic anisotropy is used. For example, non-attenuated LLSAWs can propagate in LT plate bonded to quartz without reflector between them [7].

The crystals of LN and LT refer to the same symmetry class, and the approach previously applied to LT/quartz can be implemented to find non-attenuated LLSAWs in LN/quartz. LN (symmetry *3m*) and quartz (symmetry *32*) refer to the same class in terms of elastic symmetry. One of the BAWs propagating in YZ plane of both crystals is polarized along X-axis and uncoupled with two other BAWs polarized in YZ plane. Hence, if LN plate and quartz substrate orientations are defined by the Euler angles (0°, Θ, 90°), with the sagittal plane parallel to the YZ plane of both crystals, only sagittally polarized shear BAW couples with longitudinally polarized wave. In addition, due to symmetry of LN crystal, coupling of the longitudinal (quasi-longitudinal, in general case) BAW with electrostatic potential also achieves maximum in YZ plane.

Fig. 1 shows the velocities of limiting BAWs ($V_{B1\text{-}Q}$, $V_{B2\text{-}Q}$, and $V_{B3\text{-}Q}$) in quartz substrates defined by the Euler angles (0°, Θ, 90°), where $V_{B2\text{-}Q}$ refers to the pure shear BAW polarized along X-axis. For comparison, the limiting velocity $V_{B3\text{-}LN}$ of the longitudinal BAW in (0°, Θ, 90°) cuts of LN is also shown. In LN longitudinal BAWs propagate faster than in quartz.

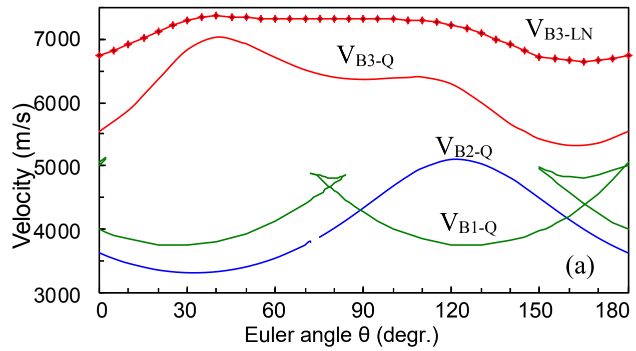

Fig. 1. Limiting velocities of three BAWs in quartz ($V_{B1\text{-}Q}< V_{B2\text{-}Q}< V_{B3\text{-}Q}$) in (0°, Θ, 90°)-quartz and longitudinal limiting BAW velocity $V_{B3\text{-}LN}$ in (0°, Θ, 90°)-LN, as functions of the angle Θ.

Though the energy of a limiting BAW is parallel to the substrate surface, usually such BAW does not satisfy mechanical and electrical boundary conditions on the surface. However, in some selected crystal orientations the stress-free mechanical boundary conditions can be fulfilled. Such *exceptional* BAW [9] can give rise to a low-attenuated LSAW branch if it is fast shear, or a low-attenuated LLSAW branch if it is longitudinal [10, 11]. Longitudinal exceptional waves exist only in few known crystals with strong elastic anisotropy [12-14], and quartz is one of these crystals. Exceptional BAW exists in certain crystal cut when the determinant of mechanical boundary conditions Det(μ_{ij}) vanishes, where $\mu_{ij}=c_{ijkl}u_k n_l$; $\boldsymbol{n}$ and $\boldsymbol{u}$ are unit vectors along propagation direction and polarization of the analyzed limiting BAW, respectively, and c_{ijkl} is the elastic stiffness tensor.

In quartz, the longitudinal BAW becomes exceptional in (0°,15.8°,90°), (0°,47.8°,90°), (0°,105.8°,90°) and (0°,137.8°, 90°) cuts [11]. Electrical boundary conditions can perturb the wave nature, but variation of Det(μ_{ij}) around zero means that low-attenuated LLSAWs can exist in quartz substrate loaded by a thin LN plate.

Fig. 2 shows an example of the slowness surfaces for LN and quartz cuts rotated according to the specified Euler angles. SAW solution at fixed velocity V involves two partial waves in the LN plate of finite thickness, with wave vectors k_{LN}^+ and k_{LN}^-, and the one mode in quartz (k_Q^+), which is responsible for energy leakage into the substrate. In each material, one of the BAWs (dotted lines) is not radiated for the analyzed orientations due to symmetry.

While the leakage into the substrate depends on the quartz orientation, the coupling coefficient k^2 in LN/quartz is dominated by the LN cut. Fig. 3,a shows the velocities of three BAWs in the YZ plane of LN calculated with the piezoelectric effect and without it, as functions of the propagation angle with the Y axis. The difference ΔV resulting from the piezoelectric effect characterizes the BAW coupling as $k^2 \approx 2\cdot\Delta V/V$. The polar diagram in Fig. 3,b refers to k^2 of the longitudinal wave in the YZ cut of LN. The maximum k^2 occurs when the BAW propagates along the direction Y+33° and the normal to the LN surface is parallel to Z+33°. Such a SAW orientation is described by the Euler angles (0°, 33°, 90°). This estimation does not take into account the beam steering angle, which may be large in quartz. More accurate simulations show that the optimal LN cut for achieving the highest electromechanical coupling of the longitudinal leaky SAW is close to (0°, 45°, 90°).

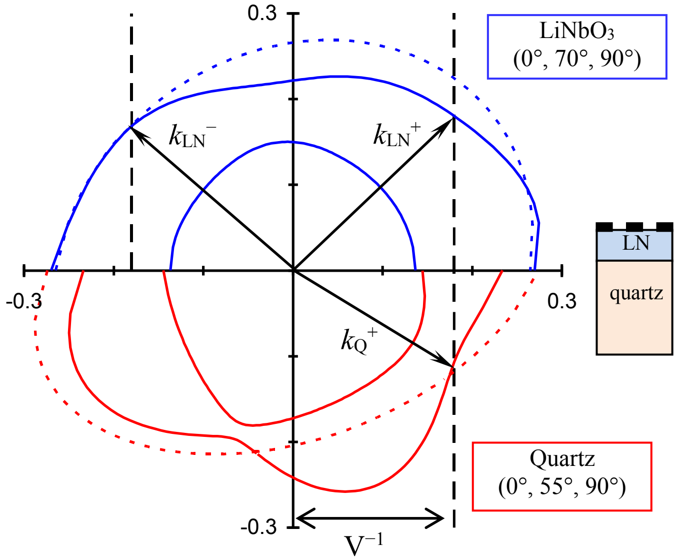

Fig. 2. An example of cross-section of the slowness surfaces by the sagittal plane: (0º, 70º, 90º)-LN and (0º, 55º, 90º)-quartz combined in the bonded wafer. Two BAWs in LN with wave vectors k_{LN}^- and k_{LN}^+ and one BAW in quartz with wave vector k_Q^+ are involved in leaky SAW solution with velocity V. Dashed lines refer to SH-polarized BAWs uncoupled with electric fields in both crystals.

For a fixed LN orientation (0°, 45°, 90°) enabling high k^2, rigorous investigation of longitudinal leaky SAW characteristics was performed in LN/quartz with Cu electrode thickness of 0.05 λ and variable cut angle of quartz substrate. Computations were made using the numerical technique SDA-FEM-SDA, which combines the finite element modeling (FEM) analysis of electrodes with the spectral-domain analysis (SDA) of a multilayered substrate [15]. The admittance functions of SAW resonators built on LN/quartz were simulated and the complex SAW velocities $V_R = 2pf_R\cdot(1+j\delta_R)$ and $V_A = 2pf_A\cdot(1+j\delta_A)$ were extracted from these functions at the resonant f_R and anti-resonant f_A frequencies, respectively. The found propagation losses at the resonance (δ_R) and the anti-resonance (δ_A) were transformed into the Q-factors of the SAW resonators associated only with leakage into bulk waves. Other loss mechanisms (electrode resistance, viscous losses, etc.) were ignored.

The minimum achievable attenuation was estimated for each Θ via the variation of the LN thickness in the interval h_{LT} = (0.35 - 0.55) λ, where λ=2p and p is the periodicity of the grating. Fig. 4 shows the minimum δ_R as a function of the Euler angle Θ. With the LN thickness changing continuously within four different ranges, $\delta_R < 10^{-3}$ was found in each range. Such low attenuation coefficients were obtained for quartz orientations of (0°, 7.5°, 90°), (0°, 42.5°, 90°), (0°, 84.5°, 90°) and (0°, 126°, 90°), which look as previously mentioned exceptional wave cuts perturbed by the effect of LN plate loaded on quartz surface.

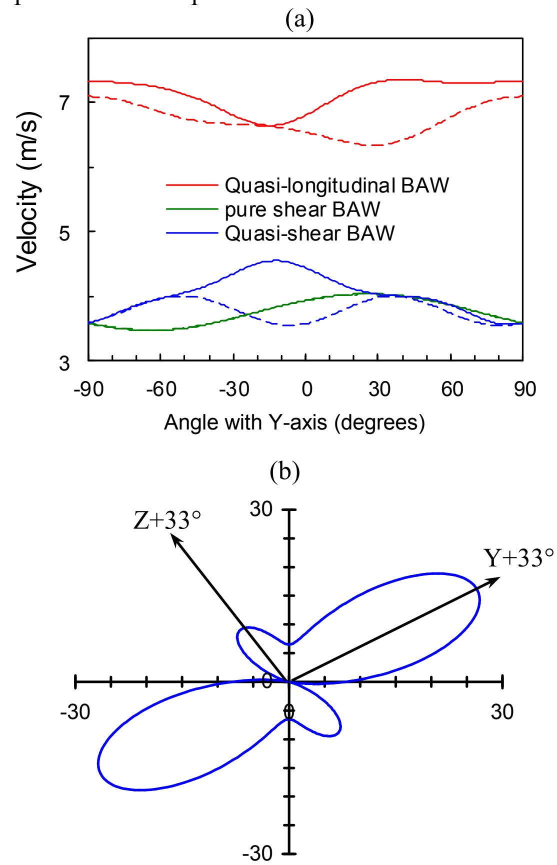

Fig. 3. BAW velocities in YZ-cut of LN, obtained without (dashed lines) and with (solid lines) piezoelectric effect taken into account, as functions of angle with Y-axis (a) and polar diagram of effective coupling k^2 in YZ plane estimated for longitudinal BAW (b).

In each of the analyzed intervals of the LN thickness, the minimum leakage occurs at a certain point in the two-dimensional space (h_{LN}, Θ). It is typical for the high-velocity leaky waves previously observed in ZnO/diamond, ZnO/ sapphire [16] and recently in ScAlN/sapphire [17].

Minimum attenuation at resonant and anti-resonant frequencies occurs at different points of the 2D space (h_{LN}, Θ). To provide low propagation losses at both frequencies in the same LN/quartz substrate, variation of duty factor of electrode structure can be used. For example, Fig. 5,a,b shows V_R, V_A, δ_R and δ_A as functions of the duty factor in (0°, 70°, 90°) LN/ (0°, 55°, 90°) quartz with h_{LT}=0.4 λ. In the analyzed interval of duty factors LLSAW velocity at resonance varies between 5400 m/s and 5700 m/s, and k^2 reaches 15.5%. The Q-factor exceeds 7000 at the anti-resonance when a/p < 0.48 and at the resonance when a/p > 0.65. Three simulated admittances shown in Fig. 6 refer to maximum Q_R, maximum Q_A and $Q_R \approx Q_A$. The wave structure at resonant frequency is illustrated by the colored diagrams of tangential (u_1) and normal (u_3) displacements. SH displacement u_2=0 due to symmetry.

In the optimal structures, the required plate and electrode thicknesses are 0.4λ and 0.05λ, respectively, or 0.44 μm and 550 A at 5 GHz. It is compatible with existing technologies and allows fabrication of high frequency SAW resonators. Due to the symmetry of the analyzed orientations the response is spurious-free in a wide range of frequencies, with the nearest spurious mode at 0.61f0.

III. CONCLUSIONS

A method, which combines symmetry consideration of plate and substrate materials with rigorous simulation of admittance functions of LLSAW resonators was applied to LN/quartz and allowed to find non-attenuated high-velocity SAWs with high coupling suitable for application in wideband high frequency high performance SAW filters.

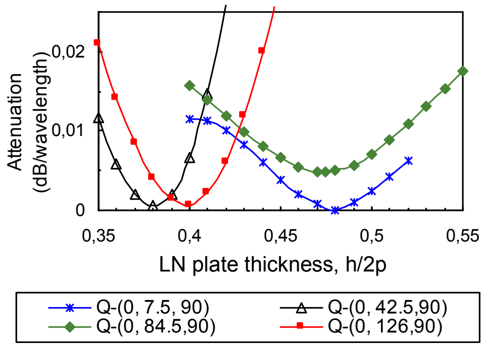

Fig. 4. Attenuation of leaky SAW as function of the normalized LN plate thickness h/2p in (0º, 45º, 90º)-LN bonded to (0, θ, 90)-quartz. Four analyzed quartz orientations enable propagation of low-attenuated HVSAW.

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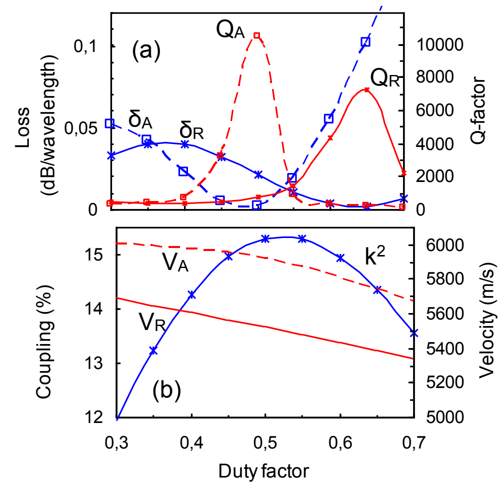

Fig. 5. Characteristics of HVSAWs in (0°, 70°, 90°)-LN / (0°, 55°, 90°)-quartz, as functions of duty factor: (a) propagation losses and Q-factors estimated at resonance (Q_R) and anti-resonance (Q_A); (b) coupling k^2 and velocities (V_R and V_A). LN plate and Cu electrode thicknesses are 0.4λ and 0.055λ, respectively.

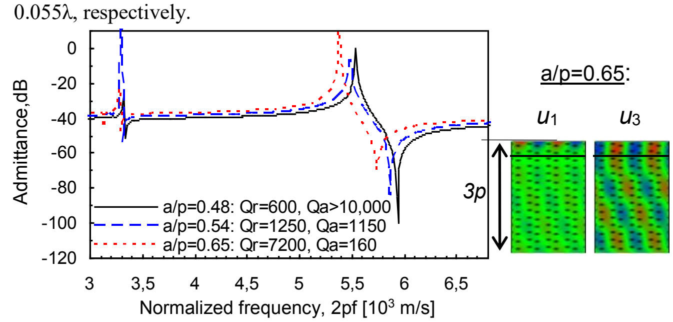

Fig. 6. Simulated admittance functions of Cu grating on (0°, 70°, 90°)-LN / (0°, 55°, 90°)-quartz for three values of duty factor optimized for maximum Q-factor at resonance or anti-resonance or maximum average Q-factor. Colored plots show displacements u_1 and u_3 at resonance when a/p=0.65.

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